Nuclear Energy University Programs

Safety and Licensing: Uncertainty Quantification

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Overview

- NEET and NEAMS
- Overview of NEAMS
- Verification Validation and Uncertainty Quantification as an element of Crosscutting Methods and Tools
- FY12 NEAMS and NEUP VU Scope
- Expectations and Deliverables

Funding and Programmatic Overview

- Nuclear Energy Enabling Technologies (NEET)
  - Crosscutting Technologies
    - Modeling and Simulation
- Nuclear Energy Advanced Modeling and Simulation (NEAMS)
  - Supporting Elements
    - Validation & Verification and Error Uncertainty Quantification
- In FY 2012 NEAMS will be supported by NEET

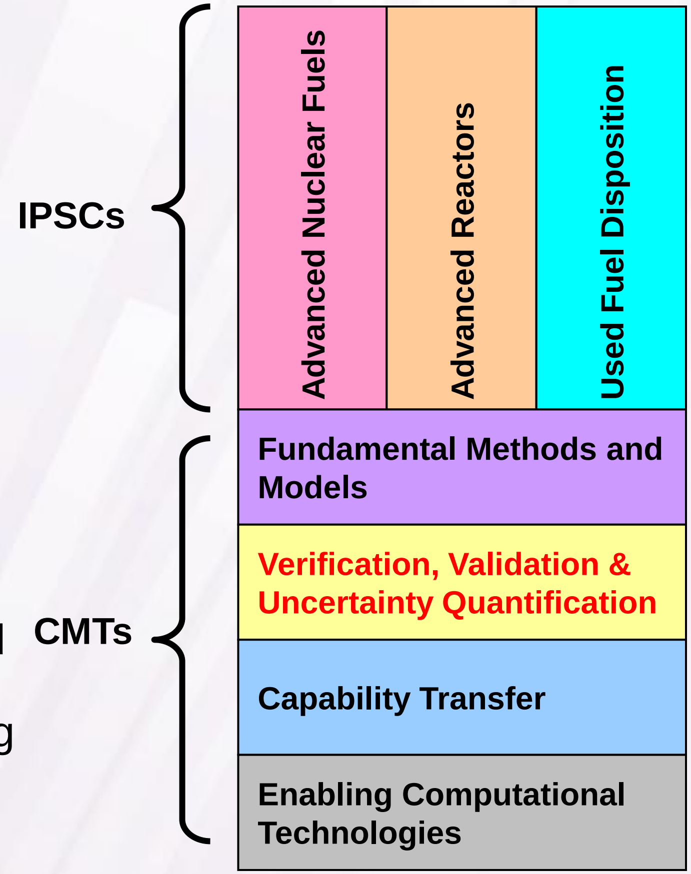
Purpose of NEAMS

Produce and deliver computational tools to designers & analysts that *predict behavior* in relevant operating regimes, particularly beyond the test base.

NEAMS Program Elements

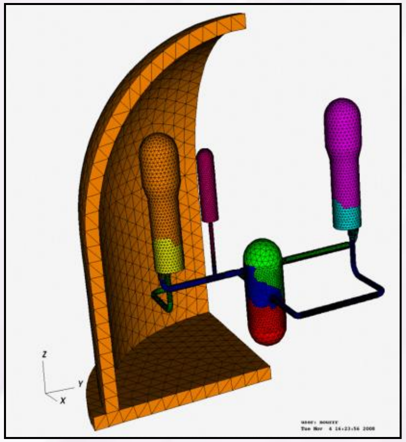
- **Integrated Performance and Safety Codes**
  - Continuum level codes that will **predict** the **performance** and **safety** of nuclear energy systems technologies
  - Attributes include 3D, science based physics, high resolution, integrated systems
  - Long-term development horizon (~10 years)
  - Codes with verification, validation and error uncertainty quantification
  - Using interoperability frameworks and modern software development techniques and tools

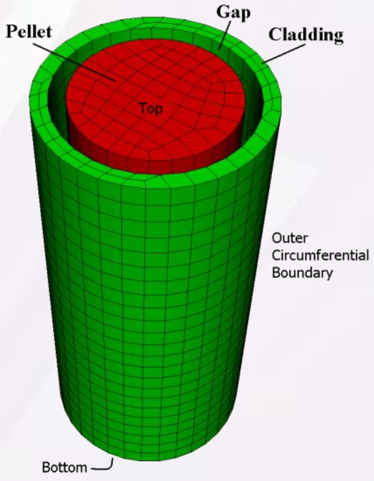
- **Crosscutting Methods and Tools**
  - Develop crosscutting (i.e. more than one IPSC) required capabilities
  - Provide a single NEAMS point of contact for crosscutting requirements (e.g. experimental data, computer technologies)
  - Smaller, more diverse teams to include laboratories, universities and industries.
  - “Tool Development” with shorter timelines



Advances Offered by NEAMS

- **Framework for organizing and managing large amounts of information**
  - Input, data management, output visualization – billions of data elements
- **FE Meshing tools for spatial representation**
  - Automated mesh generation, mesh translation between codes, properties
  - Directly from CAD files, often
  - Flexible resolution: highly localized (fine mesh), large volume (coarser mesh)
- **Modern, sophisticated equation solvers**
  - Coupled neutron, thermal-fluid, thermal-mechanics fields (“multi-physics”)
- **High-performance computing platforms for understanding difficult problems**
  - Massively parallel, 100,000s of cores
- **Verified upon release**
  - Tools for automated verification
- **Advances in uncertainty quantification**
- **Expertise from the ASC (NNSA) and SciDAC (Office of Science)**





What are Verification, Validation, and Error Uncertainty Quantification?

- **Verification: Are the requirements *implemented correctly*?**
  - *Are we solving the equations correctly?*
  - *Are we solving the equations to sufficient accuracy?*

- **Validation: Is the code representative of the real world?**
  - *Are we solving the right equations?*
  - *Are the requirements correct?*

- **Error Uncertainty Quantification: The end-to-end study of the *reliability of scientific inferences*.**
  - *Uncertainty and error affect every scientific analysis or prediction.*

Collectively known as "VU"

What Will VU Do?

- **Verification: Develop test problems, new methods, and software tools to quantify error**

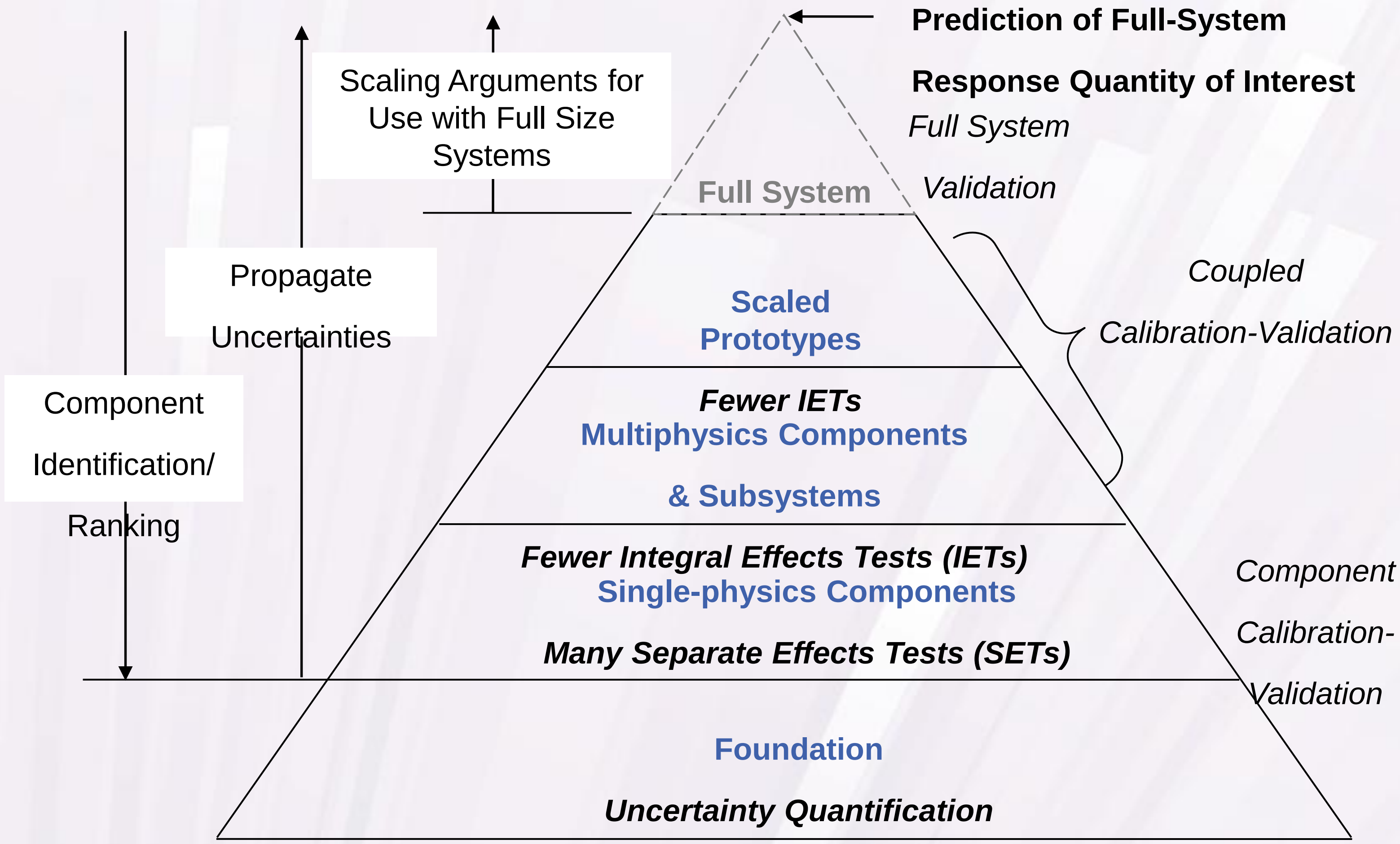
- **Validation: In conjunction with IPSCs and R&D campaigns, assess validation datasets and identify database gaps as required by the VU-assessed and licensing missions**

- **Calibration, Sensitivity Analysis (SA), UQ: Develop and deploy new capabilities and software tools for the NEAMS IPSCs**

- **Licensing: Serve as the primary interface to the NRC for support of licensing using NEAMS capabilities**

What will VU do for each IPSC?

Validation Pyramid: Part of an IPSC V&V Plan



More on "Credibility"

- **Credibility is related to *Predictive Maturity***
  - Can this be measured?
- **Elements of Predictive Maturity**
  - Geometry fidelity, Physics model and algorithm fidelity, Code verification, Solution verification, Validation coverage and discrepancy, UQ/SA, Documentation, others?
- **Some Attempts to Quantify**
  - Predictive Capability Maturity Model (PCMM), *SNL*
  - Predictive Maturity Index (PMI), *LANL*
  - Credibility Assessment Scale (CAS), *NASA*

Can we apply this concept to the NEAMS IPSCs?

NEAMS VU Scope in FY 2012

- **IPSC Support**
  - Provide consulting support to the IPSCs in implementing their specific V&V plans
  - Provide support for supporting verification studies and UQ and sensitivity analyses for selected software
  - Expansion of the concept of the Predictive Capability Maturity Model (PCMM) into more NEAMS-specific VU-assessment tables and their use the tables to develop initial VU assessments for one or more IPSCs
- **Bayesian Methodology Development**
  - Parameter sampling techniques
  - Investigate sequential experimental design strategies for data collection from multiple models and experiments
  - Investigate particle filtering (sequential Monte Carlo) approaches
- **Predictive Maturity Development**
  - Investigate model-form effects

FY12 NEUP VVUQ Scope

- Development of phenomena-based methodology for Uncertainty Quantification:
  - Propagating uncertainties through inter-fidelity multi-scale physics models “upscaling”
  - Parameter sensitivities and uncertainties in tightly-coupled multi-physics models
  - Interpretation of large experimental data sets
  - Design and develop experiments at various scales for model validation of mathematical uncertainty propagation approach

VU is an integral part of the goal to develop computational tools that are an accurate reflection of reality, predictive and an area that can greatly benefit from university collaboration

Expectations and Deliverables

- **Mission-driven expectations**
  - 20% relevance
  - 80% technical

- **Deliverables clearly tied to IPSCs/Campaigns and identified in proposals**
  - Specific
  - Measurable
  - Achievable
  - Realistic
  - Time-bound

- **Performance feedback**

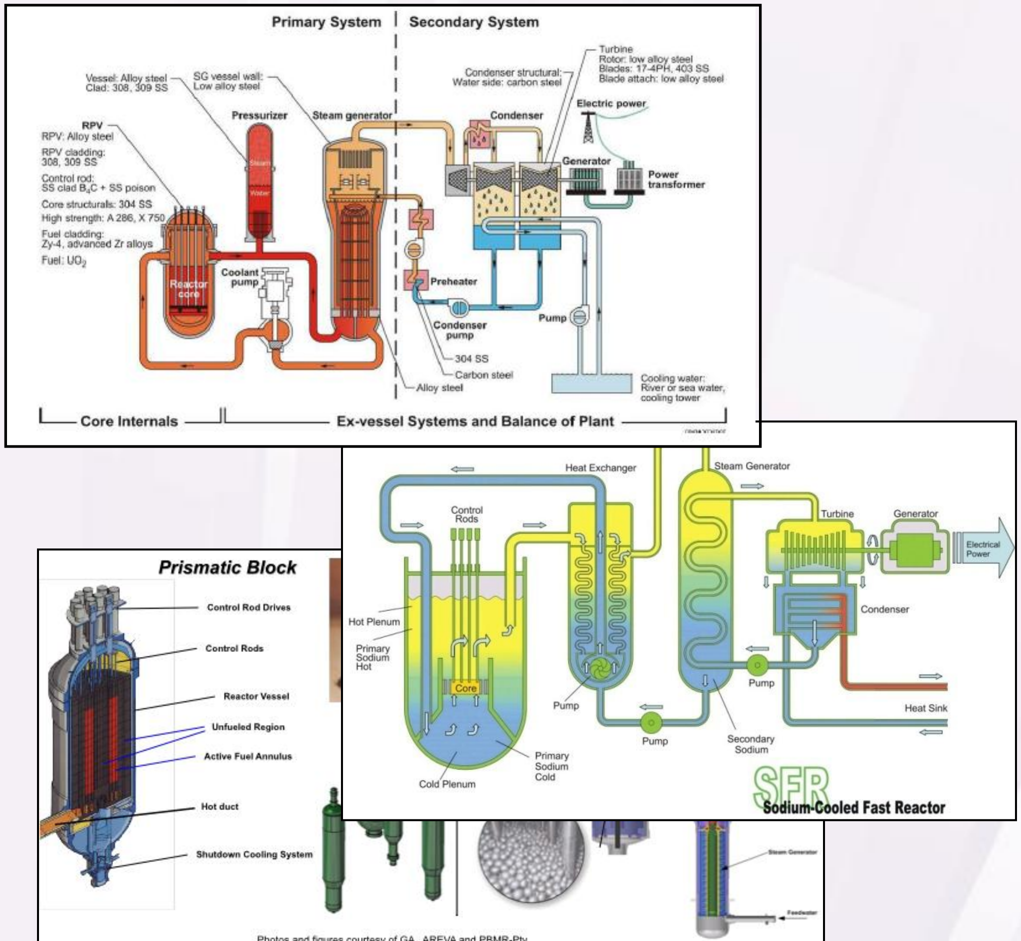
Backup Slides

Predictive Capability Maturity Model (PCMM)

(Version 1: Oberkampf, Pilch, and Trucano; 2007)

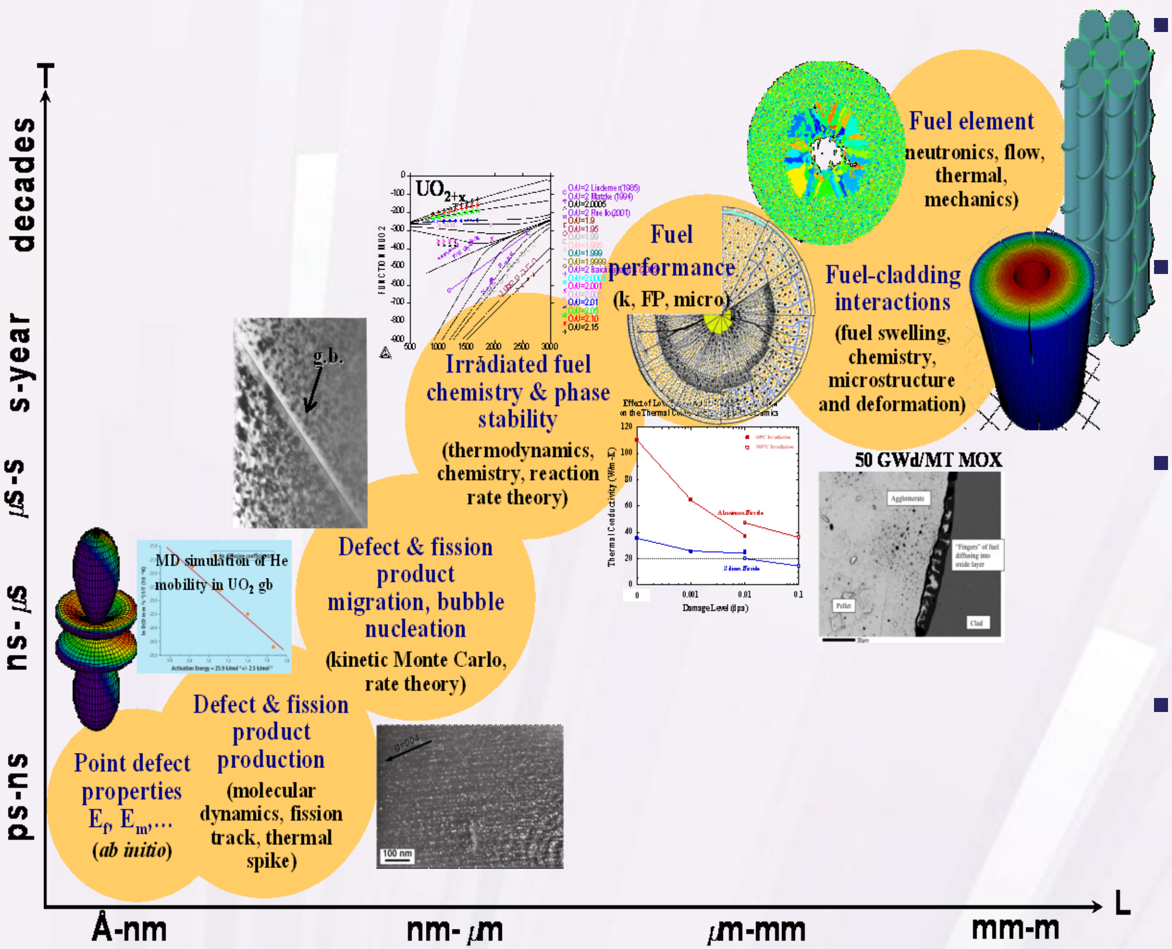
ELEMENT \ MATURITY	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g., Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g., Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g., Qualification Support	Maturity Level 3 High-Consequence, Decision Making Based on M&S, e.g.. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and boundary conditions (BCs)	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built," e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate-effects tests (SETs) and integral-effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&Cs) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated, and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive SAs conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

Reactor Integrated Performance and Safety Code



- **Scope**
  - Modeling and simulation capabilities to <u>predict</u> the performance and safety of:
    - **Existing LWR**
    - **Newly deployed LWRs**
    - **Advanced Reactors**
      - **SMR**
      - **VHTGR**
      - **Fast Reactors**
  - Initial focus has been on SFRs in support of Fuel Cycle R&D
  - Work also underway on codes for LWR (R7 for RISMC) and VHTR

Nuclear Fuels Integrated Performance and Safety Code



- **Scope**
  - Develop coupled 3D computational tool to predict performance of nuclear fuel pins and assemblies, applicable to both fuel design and fabrication
  - Develop multi-scale, multi-physics framework with appropriate scale bridging techniques
  - Develop atomistically informed, predictive meso-scale microstructure evolution model that can be bridged to the engineering scale
  - Develop with flexibility of application to nuclear fuels for all reactor types (gas, light water, liquid metal)